145b Solving Mass Transfer Problems on the Computer Using Mathcad

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The author has a longtime interest in the use of the computer in chemical engineering computation. In the past, many of these computations were very time consuming. Today, the computer can be used to rapidly and accurately make these computations. Many of these problems were traditionally solved by hand using graphical means. The great advantage of the graphical techniques is that they provide a picture of the occurring phenomena. As a teaching tool this was indispensable. However, the graphical solutions were often very approximate and took a great deal of time and effort. The author has written several hundred routines in Chemical Engineering, with an emphasis on graphics and iterative computations. “Mathcad” was the software of choice because no writing of code was necessary and the graphics produced were superb. Often the programs written were capable of solving the problem completely. For example, the binary distillation program can be used to completely design the column. It could also provide graphics that could be supplied to students, so that they could generate their own graphical solutions to the engineering problem. For example, in binary distillation xy and txy diagrams are available for about 60 different binary systems, using Wilson or NRTL equations. These may be copied and distributed to students in order to teach the McCabe-Thiele procedure. The computer solution to the problem is capable of solving it completely. It can deal with details such as minimum (even if an enriching section pinch occurs) and total reflux. For a specified reflux ratio the program can obtain the number of ideal stages and the optimum feed location. Since the program is provided with a routine for obtaining the Murphree stage efficiency for each ideal stage, real stages can be (with appropriate graphical output) handled. It will also deal with the column diameter. The effect of compositions, reflux ratio and feed condition can be readily demonstrated to beginning students. If the equilibrium information is provided as experimental txy data, programs are available, using Barker's method to find the Wilson or NRTL parameters. Systems that are pseudo-binary such as acetic acid and water can in many cases be treated. These programs will plot the experimental data points and the resulting smoothed curve on the same graph. This allows the user to see immediately the quality of the fit. One special program in continuous binary distillation solves the separation of n-butanol from water, which requires two columns and a decanting tank to separate the heterogeneous liquids. A few enthalpy-concentration diagrams have been generated which has made it possible to perform Ponchon-Savarit calculations. The graphical outputs have been printed on legal sized paper in order to have room for the delta points. Enthalpy-concentration diagrams without the distillation can be printed for distribution to students. In addition to continuous binary distillation, programs have been written for binary batch distillation. These were written for constant reflux ratio with variable distillate composition and for constant distillate composition and variable reflux ratio. These are provided with animation to demonstrate the sequence of conditions with time with a specified number of ideal stages and a specified initial charge composition. Continuous multi-component distillation is also represented. These use the K values presented in “Equilibrium Staged Separations” by Wankat on page 26. Programs that will solve sharp or sloppy separations have been written. One demonstration program solves a system with four hydrocarbon components, with a sharp separation using both the Wang and Henke technique (without energy balances) and the Fenske-Underwood-Gilliland technique. The results compare very favorably. Most recently azeotropic distillation has been programmed. Two systems have been examined. These are water, ethanol using benzene as the entraining agent and water, ethanol using toluene as the entraining agent. The ternary Wilson equation was used was used for the constant pressure vapor-liquid equilibrium. Curve fitting was used to obtain the liquid-liquid equilibrium. Although these programs work, this is still a work in progress. Alternate methods for expressing the equilibria are being examined. The use of packed towers in gas absorption has been examined. The old procedures involved graphical plotting to find the equilibrium mole or mass fractions. Data was prepared in tabular form so that a graphical integration could be performed in order to obtain the packing height. This procedure was a slow, time consuming operation. The computer alternate involves punching in equilibrium data, and

using the available computer regression fit for the data. An equation for the equilibrium values of y as a function of x can be obtained. This is not difficult because the data is often nearly linear. The equation for the height of the packing may be solved by integration between limits on the computer. Countercurrent liquid extraction was examined. Some of the results were presented in August of 2004 in Prague in the Czech Republic at Karlovy University. Six different systems were shown (still more are on the machine). Four of the systems were of the type where two binary pairs are completely miscible and only one binary pair has immiscibility. Such a system will have a plait point. The programs for these systems simulated countercurrent extraction. Two other systems, each having but one binary pair of components completely miscible were also used. These systems do not have a plait point. For these systems counter-current extraction with reflux was used. Known example problems from the literature were chosen for these, in order to show that the procedures worked correctly and give correct results. These were the extraction of styrene from ethyl benzene using ethylene glycol and the other was the extraction of oleic acid from cottonseed oil using liquid propane at 98.5 C and 625 psia. Both of these programs involved the use of a solvent free basis. In all of the extraction problems an xy diagram was computer generated showing the equilibrium curve, a curved operating line and the ideal stages.